

Monday, May 23 2005

8:30	Opening and Welcome
Session 1 : First Principles and Other Matters Chair : Jan VREŠTÁL = = = Zi-Kui LIU	
8:40	<i>Z-K. Liu</i> Stability, Metastability, and Instability: on Integrating First-Principles and CALPHAD modeling
9:10	<i>R.N. Nogueira and C.G. Schön</i> Embedded Atom Study of the interaction between point defects in iron aluminides
9:30	<i>M. Šob, M. Friák, D. Legut, M. Čák, T. Káňa and M. Zelený</i> Ab initio studies of displacive phase transformations in metallic systems
9:50	<i>J. Houserová and M. Šob</i> Ab initio lattice stability in Laves phases: all-electron (WIEN) vs. pseudopotential (VASP) calculations
10:10	Coffee
10:40	<i>B-J. Lee</i> Semi-Empirical Interatomic Potentials for Carbon and Fe-C System
11:00	<i>S. Prins, R. Arroyave and Z-K. Liu</i> The use of first principle calculations for the thermodynamic modeling of B2 in the Al-Ni-Ru system
11:20	<i>T. Tokunaga, H. Ohtani and M. Hasebe</i> Thermodynamic analysis of the Zr-Be system using thermochemical properties based on <i>ab initio</i> calculations
11:40	<i>V.L. Vinograd, M.H.F. Shuiter and B. Winkler</i> The Impurity Method and its applications to oxide solid solutions with coupled substitutions
12:00	<i>A.N. Grundy, B. Hallsted, and L. J. Gauckler</i> Calculating Defect Chemistry using the CALPHAD Approach
12:30	Lunch

Session 2 : High Pressure Chair : Josep Lluís TAMARIT = = = Olga FABRICHNAYA	
14:00	<i>O.Fabrichnaya, S. Lakiza, M. Zinkevich and F. Aldinger</i> Thermodynamic database for the ZrO ₂ -Gd ₂ O ₃ -Y ₂ O ₃ -Al ₂ O ₃ system
14:30	<i>A.E. Gheribi, J. Rogez, J.C. Mathieu, F. Marinelli and M.C. Record</i> Theoretical calculation of phase diagram : Introduction of the pressure dependance
14:50	<i>M.H.G. Jacobs, B.H.W.S. de Jong, A.P. van den Berg and H.A.J. Oonk</i> Thermo-physical properties and phase equilibria of mantle materials derived from lattice vibrations
15:10	<i>A.P. van den Berg, M.H.G. Jacobs and B.H.W.S. de Jong</i> Thermal Convection Models for Planetary Mantles Based on Self-consistent Thermodynamics
15:30	Posters – Coffee

Session 3 : Modeling and Experiments Chair : Jean-Claude GACHON = = = Rainer SCHMID-FETZER	
16:40	<i>R. Schmid-Fetzer, M. Ohno, and D. Mirkovic</i> Thermodynamic Modeling and Key Experiments in Mg-Al-Mn-Zn Alloys
17:10	<i>M. Medraj, M.A. Parvez, E. Essadiqi, A. Muntasar and G. Dénès</i> Experimental Investigation and Thermodynamic Modeling of Magnesium Alloy Systems
17:30	<i>M. Abou Khatwa and D.V. Malakhov</i> On the stability of the α -phase in aluminum alloys
17:50	<i>S. Balanetskiy, T.Ya. Velikanova, B. Grushko, M. Feuerbacher and K. Urban</i> Formation and stability of complex intermetallic phases in the Al-rich region of Al-Pd-Re and Al-Pd-Mn
18:10	<i>J. Vizdal and A. Kroupa</i> The experimental and theoretical study of phase equilibria in the Bi-Sn-Zn system
20:00	Dinner

Tuesday, May 24 2005

Session 4 : CALPHAD Thermodynamics	
Chair : Nathalie DUPIN = = = Patrice CHARTRAND	
8:30	<i>P. Chartrand</i> Thermodynamic Modeling of MgF ₂ - MgO in NaF - AlF ₃ - Al ₂ O ₃ - CaF ₂ - LiF
9:00	<i>L. Kaufman</i> (CT) The CALPHAD Approach to Computational Thermodynamics
9:30	<i>J. Vrestal, J. Pinkas, A Kroupa , J. Houserová, A. Scott and A. Watson</i> Thermodynamic Assessment of Phase Diagram of Bi-Pd System
9:50	<i>T. Abe, M. Shimono and H. Onodera</i> Thermodynamic modeling of the undercooled liquid by the regular associated solution model
10:10	Coffee
10:40	<i>T. Benlaharache, N. David, J.M. Fiorani and M. Vilasi</i> Thermodynamic modeling of the Mo-Pt, Pt-Si and Mo-Pt-Si systems
11:00	<i>J.C. Tedenac, D. Ravot and S.G. Fries</i> The behaviour of the B8, C18 and DO ₂ phases in the Co-Fe-Sb ternary system
11:20	<i>H. Ohtani, N. Hanaya, S. Teraoka, M. Abe and M. Hasebe</i> Thermodynamic analysis of the Fe-Ti-P ternary system
11:40	<i>D. Sedmidubský, J. Leitner, A. Strejc, O. Beneš and M. Nevřiva</i> Phase Equilibria Modeling in Bi-Sr-Mn-O System
12:00	<i>B. Onderka and W. Zakulski</i> Phase Diagram Calculation of the Al-Mg-Sr System
12:30	Lunch

Session 5 : Kinetic Matters	
Chair : Hyuck Mo LEE = = = Bengt HALLSTEDT	
14:00	<i>B. Hallstedt</i> Melting of Alloys
14:30	<i>J. Bratberg, J. Ågren and K. Frisk</i> Diffusion simulations of MC and M ₇ C carbide coarsening in bcc and fcc matrix using a new thermodynamic and kinetic description
14:50	<i>M. Palumbo, M. Baricco and L. Battezzati</i> Thermodynamic and kinetic modeling of the Fe-B and Al-Ni-Ce amorphous and nanocrystalline alloys
15:10	<i>N. Moelans, B. Blanpain and P. Wollants</i> Phase field simulations of grain growth in materials containing a finely dispersed second phase
15:30	Posters – Coffee
16:40	<i>R. R. De Avillez, F. C. Rizzo Assunção and B. Marinkovic</i> Aging Behavior of a 2.25Cr-1Mo Steel
17:00	<i>R. Bernst, G. Inden and A. Schneider</i> Carburisation of diffusion couples
17:20	<i>M. Sacerdote-Peronnet and J.C. Viala</i> Observed reaction paths and corresponding diffusion paths in ternary metallic phase diagrams
17:40	<i>A. Davydov, K. Moon, W. Boettinger and U. Kattner</i> Use of the Au-Zn-O phase diagram for ZnO nanowhisker growth
18:00	<i>J. Moon, J. Ryu, C. Lee, Y. An and J. Lee</i> Development of prediction model for precipitates kinetics and austenite grain growth in the weld heat affected zone
20:00	Dinner

Wednesday, May 25 2005

Session 6 : Miscellaneous	
Chair : Pierre PERROT = = = Arthur PELTON	
8:30	<i>A.D. Pelton</i> Models for multicomponent liquid solutions
9:00	<i>S.S. Han, J.K. Kang, H.S. Kim, J.Y. Lee, A C T. van Duin , W.A. Goddard III and H.M. Lee</i> Hydrogen adsorption and desorption mechanism in carbon nanotubes
9:20	<i>P. Koukkari, R. Pajarre and K. Penttilä</i> Calculation of Constrained Equilibria by Gibbs Energy Minimisation
9:40	<i>B. Guy</i> The qualitative structure of phase diagrams: from the works of Schreinemakers (the Netherlands, beginning of the XX th century) to present day
10:00	Coffee
10:30	<i>A.Yu. Zakharov, M.A. Zakharov, A.L. Udovsky and H.A.J. Oonk</i> On the statistical thermodynamics of solutions with variable valence states of one of the components
10:50	<i>O. Semenova, H. Numakura and H. Ipser</i> Ni ₃ Ga – Defect Structure and Changes in Degree of Long Range Order
11:10	<i>J-M. Joubert</i> Crystallochemistry and CALPHAD modeling of the σ phase
11:30	<i>C-I. Huang, Y-C. Chiu and Y-C. Hsu</i> Phase Behavior of a Diblock Copolymer in the Presence of Two Solvents
11:50	<i>Z. Moser, W. Gąsior and J. Pstruś</i> Influence of antimony additions on surface tension and density of Sn-Sb, Sn-Ag-Sb and Sn-Ag-Cu-Sb alloys. Experiment vs. modeling
12:10	<i>L. Kaufman and M. Bamberger</i> Introduction to CALPHAD XXXV (2006), Haifa, Israël
12:25	End of Session
12:45	Lunch and Excursion
19:00	Conference diner in Chateau Neercanne

Thursday, 26 May 2005

Session 7 : Experimental Thermodynamics	
Chair : Miquel Àngel CUEVAS-DIARTE = = = Susan MESCHEL	
8:30	<i>S.V. Meschel and O.J. Kleppa</i> The Standard Enthalpies of Formation of Some Inter- Transition Metal Compounds by High Temperature Direct Synthesis Calorimetry
9:00	<i>G.C. Coelho, J.C. Gachon, C.A. Nunes, J.M. Fiorani and M. Vilasi</i> Enthalpies of formation of intermetallic phases of the Ti-Si, Ti-B and Ti-Si-B systems measured by direct synthesis calorimetry
9:20	<i>M. Kopyto, B. Onderka, A.T. Dinsdale and L. A. Zabdyr</i> Phase Equilibria in the Ag-Cu-Sn LEAD-Free Solder Alloys
9:40	<i>T. Markus, M. Ohnesorge, D. Kobertz and K. Hilpert</i> Thermodynamic Activity Measurements and Assessment of the System NaI – CeI ₃
10:00	Coffee
10:30	<i>A. Talekar, R. Chellappa, D. Chandra, A.O. Tsokol and J.A. Sampio</i> Low Temperature Heat Capacities and Debye Temperatures of Organic “Plastic” Crystals
10:50	<i>S.C. Divi, R. Chellappa and D. Chandra</i> Excess Molar Heat Capacities of Organic “Plastic Crystal” Binary System: Tris(hydroxymethyl)aminomethane – Neopentylglycol
11:10	<i>V.T. Witusiewicz L. Sturz, U. Hecht and S. Rex</i> Experimental Investigation and CALPHAD Description of the Quaternary Organic Alloy System AMPD-DC-NPG-SCN

11:30	<i>L. Bencze, D. Raj, T. Markus, S. Das, W. Löser, W.A. Oates, D. Kath, L. Singheiser and K. Hilpert</i> Thermodynamic Activity Measurements in the B2 Phase (Ni,Fe) _{1-x} Al _x
11:50	<i>W. A. Oates, L. Bencze, T. Markus and K. Hilpert</i> Thermodynamic Modelling of the A2/B2 Phases in the Fe-Ni-Al-Va System
12:30	Lunch

Session 8 : Nuclear Materials and Other Matters

Chair : Marko HÄMÄLÄINEN = = = Rudy KONINGS

14:00	<i>P. Masset and R.J.M. Konings</i> Optimisation of MCl-AnCl _x (M=Li,Na,K; An=U, Pu) phase diagrams
14:30	<i>C. Toffolon-Masclat, S. Chatain, C. Gueneau and N. Dupin</i> Thermodynamic study of the Zr-Fe system
14:50	<i>I. Drouelle, C. Gueneau, S. Chatain and Ph. Zeller</i> Thermodynamic Assessment of Al-Li-O-Zr System
15:10	<i>A.L. Udovsky, D.A. Vasilyev and H.A.J. Oonk</i> Thermodynamic assessments of stabilities Parameters for metastable ω-phases of Zr and U and Phase Diagram of the U-Zr system, including δ-UZr ₂ -phase
15:30	Posters – Coffee
16:40	<i>R. Jerlerud Pérez, V. Baykov, B. Sundman and C. Toffolon-Masclat</i> Reassessment of the Zr-Sn binary system
17:00	<i>J. van der Meer, R. Konings and H.A.J. Oonk</i> Thermodynamic modelling and experiments on LiF-NaF-LnF ₃ and LiF-NaF-AnF ₃ for Molten Salt Reactor fuel
17:20	<i>G.J.L.M. de Haas, R.P.C. Schram and M.J. den Exter</i> Incorporation of boron in MgO-based composites for transmutation
17:40	<i>L. Teng, R.E. Aune, W. Li, S. Seetharaman</i> Thermodynamic investigations and assessment of the Mn-Ni-C system
18:00	<i>C. Robelin and P. Chartrand</i> Modeling the Volumetric Properties of Multicomponent Liquids : The NaCl-KCl-MgCl ₂ -CaCl ₂ and Na ⁺ , Al ³⁺ , Ca ²⁺ //F ⁻ , O ²⁻ Systems
20:00	Dinner

Friday, May 27 2005

Session 9 : Cluster Variation Subjects

Chair : Marcel SLUITER = = = Tetsuo MOHRI

8:30	<i>T. Mohri and Y. Kobayashi</i> Crystal-Glass transition studied by CVM and PPM
9:00	<i>L. Eleno, J. Balun, C. Schön, G. Inden</i> CVM calculations on the bcc Fe-Rh-Ti system
9:20	<i>D.E. Nanu, S. Shang and A.J. Böttger</i> A CVM-based study of the effect of alloying on hydrogen solubility in palladium alloys
9:40	<i>S. Shang and A.J. Böttger</i> A combination of the cluster variation method and <i>ab initio</i> calculations: application to hexagonal interstitial ε-Fe ₆ N _v alloys
10:00	Coffee break

Session 10 : CALPHAD Thermodynamics and Related Subjects

Chair : Michel JACOBS = = = Suzana FRIES

10:30	<i>S.G. Fries</i> Check List for Publishing CALPHAD-type Thermodynamic and Kinetic Assessments: proposal for the CALFOR standard format
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11:00	<i>D. Lindberg, P. Chartrand and R. Backman</i> Thermodynamic modeling of the system Na-K-S
11:20	<i>S.H. Lee and K.J. Lee</i> The Effects of Alloying Elements on Thermodynamic Properties of Nb-Carbide in Microalloyed Steels
11:40	<i>M.H.F. Sluiter, V.L. Vinograd and Y. Kawazoe</i> Ab Initio Calculations on Garnet Solutions
12:00	<i>D.W. Shin and Z.K. Liu</i> Special Quasirandom Structure calculation of binary HCP alloys
12:20	Closing
12:30	Lunch